



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:20 PM GMT

PDB ID : 3TLF
Title : Crystal structure of an enoyl-CoA hydratase/isomerase from Mycobacterium paratuberculosis
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2011-08-29
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

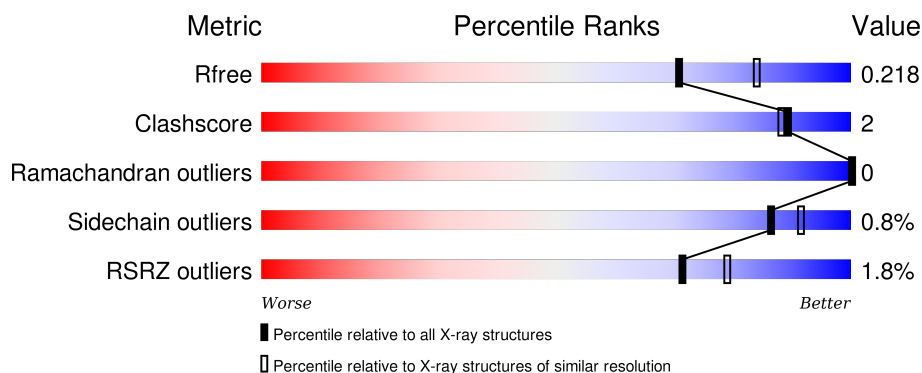
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 84%, yellow 84%, yellow 88%, orange 88%, orange 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 84% 8% 8% </div> </div>
1	B	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 86%, yellow 86%, yellow 90%, orange 90%, orange 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 3% 86% 5% 8% </div> </div>
1	C	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 84%, yellow 84%, yellow 88%, orange 88%, orange 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 84% 8% 8% </div> </div>
1	D	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 91%, yellow 91%, yellow 95%, orange 95%, orange 99%, grey 99%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 3% 91% 6% . </div> </div>
1	E	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 89%, yellow 89%, yellow 93%, orange 93%, orange 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 89% . 7% </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	274	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	C	271	-	-	-	X
2	EDO	D	272	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12753 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called enoyl-CoA hydratase/isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	1	0
			1968	1232	352	374	10			
1	B	252	Total	C	N	O	S	0	1	0
			1930	1216	346	358	10			
1	C	252	Total	C	N	O	S	0	3	0
			1966	1237	351	368	10			
1	D	266	Total	C	N	O	S	0	0	0
			2028	1273	363	383	9			
1	E	254	Total	C	N	O	S	0	0	0
			1950	1223	349	369	9			
1	F	253	Total	C	N	O	S	0	0	0
			1937	1216	346	365	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q73XB1
A	-2	PRO	-	EXPRESSION TAG	UNP Q73XB1
A	-1	GLY	-	EXPRESSION TAG	UNP Q73XB1
A	0	SER	-	EXPRESSION TAG	UNP Q73XB1
B	-3	GLY	-	EXPRESSION TAG	UNP Q73XB1
B	-2	PRO	-	EXPRESSION TAG	UNP Q73XB1
B	-1	GLY	-	EXPRESSION TAG	UNP Q73XB1
B	0	SER	-	EXPRESSION TAG	UNP Q73XB1
C	-3	GLY	-	EXPRESSION TAG	UNP Q73XB1
C	-2	PRO	-	EXPRESSION TAG	UNP Q73XB1
C	-1	GLY	-	EXPRESSION TAG	UNP Q73XB1
C	0	SER	-	EXPRESSION TAG	UNP Q73XB1
D	-3	GLY	-	EXPRESSION TAG	UNP Q73XB1
D	-2	PRO	-	EXPRESSION TAG	UNP Q73XB1
D	-1	GLY	-	EXPRESSION TAG	UNP Q73XB1
D	0	SER	-	EXPRESSION TAG	UNP Q73XB1
E	-3	GLY	-	EXPRESSION TAG	UNP Q73XB1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	PRO	-	EXPRESSION TAG	UNP Q73XB1
E	-1	GLY	-	EXPRESSION TAG	UNP Q73XB1
E	0	SER	-	EXPRESSION TAG	UNP Q73XB1
F	-3	GLY	-	EXPRESSION TAG	UNP Q73XB1
F	-2	PRO	-	EXPRESSION TAG	UNP Q73XB1
F	-1	GLY	-	EXPRESSION TAG	UNP Q73XB1
F	0	SER	-	EXPRESSION TAG	UNP Q73XB1

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		

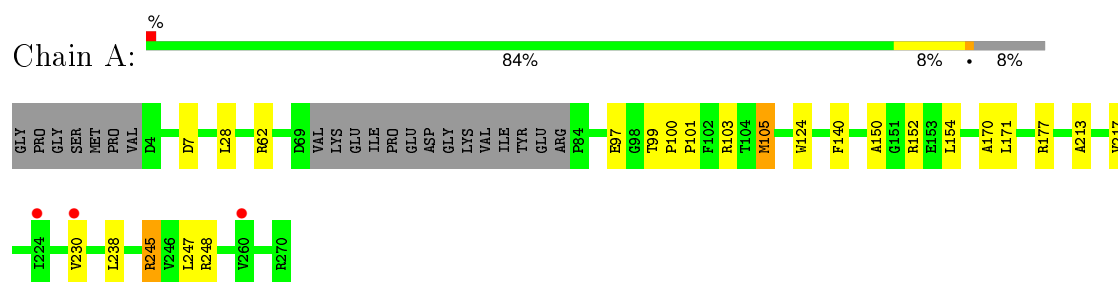
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	150	Total	O	0	0
			150	150		
3	C	145	Total	O	0	0
			145	145		
3	D	156	Total	O	0	0
			156	156		
3	E	178	Total	O	0	0
			178	178		
3	F	155	Total	O	0	0
			155	155		

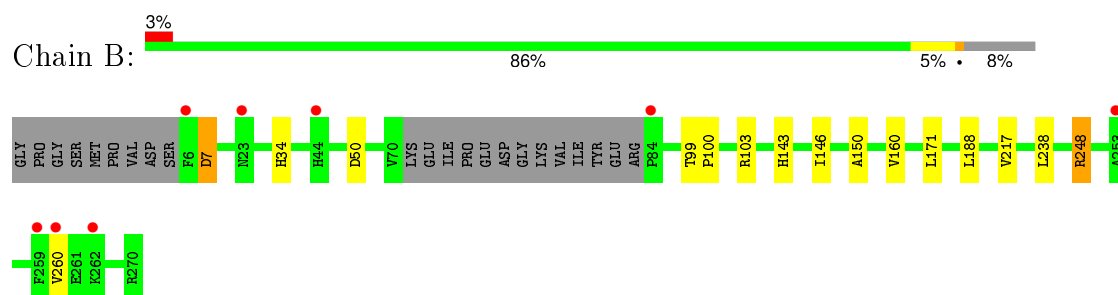
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

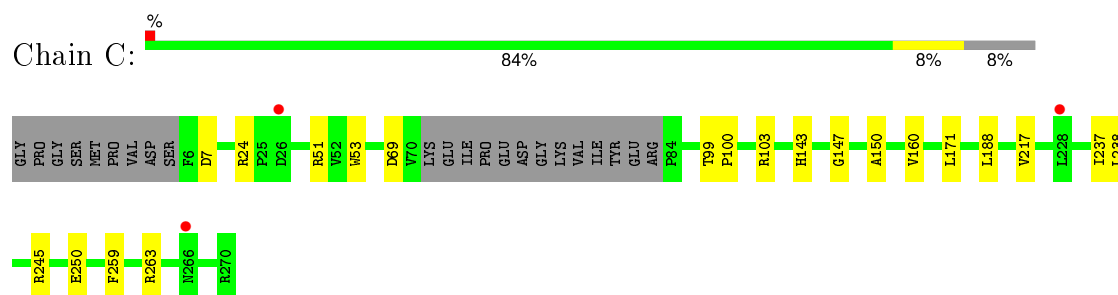
- Molecule 1: enoyl-CoA hydratase/isomerase



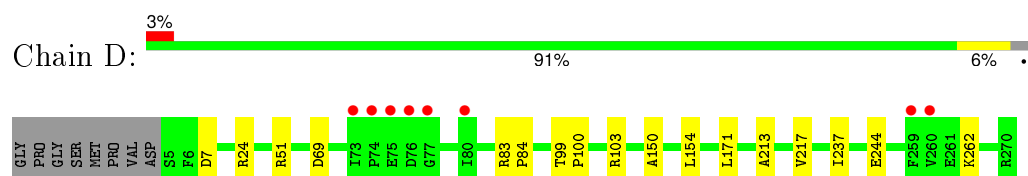
- Molecule 1: enoyl-CoA hydratase/isomerase



- Molecule 1: enoyl-CoA hydratase/isomerase



- Molecule 1: enoyl-CoA hydratase/isomerase

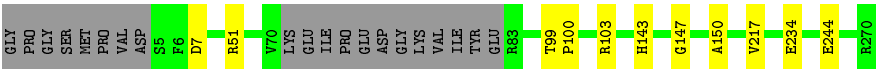


● Molecule 1: enoyl-CoA hydratase/isomerase

Chain E:

89%

• 7%



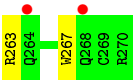
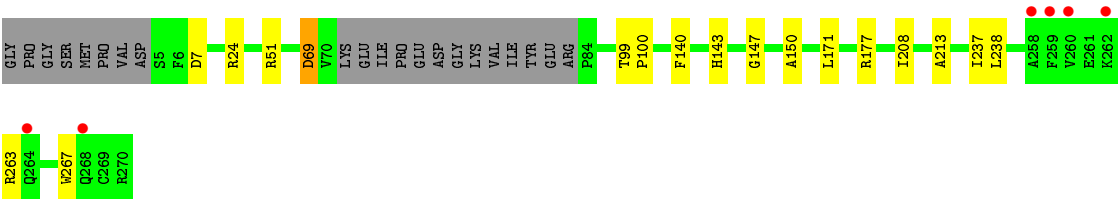
● Molecule 1: enoyl-CoA hydratase/isomerase

Chain F:

2%

86%

6% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.74Å 140.50Å 148.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 49.19 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.15) 99.0 (49.19-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.181 , 0.217 0.183 , 0.218	Depositor DCC
R_{free} test set	4427 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 88344 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12753	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	1/2010 (0.0%)	0.86	6/2732 (0.2%)
1	B	0.71	0/1972	0.78	2/2684 (0.1%)
1	C	0.74	1/2011 (0.0%)	0.82	4/2736 (0.1%)
1	D	0.77	0/2070	0.81	3/2823 (0.1%)
1	E	0.75	0/1989	0.79	4/2709 (0.1%)
1	F	0.75	1/1976 (0.1%)	0.79	2/2691 (0.1%)
All	All	0.74	3/12028 (0.0%)	0.81	21/16375 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	TRP	CD2-CE2	5.98	1.48	1.41
1	F	267	TRP	CD2-CE2	5.28	1.47	1.41
1	A	124	TRP	CD2-CE2	5.03	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	245	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	103	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	C	245	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	245	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	D	103	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	103	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	E	51	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	7	ASP	CB-CA-C	-5.79	98.82	110.40
1	E	7	ASP	CB-CA-C	-5.64	99.11	110.40
1	C	103	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	248	ARG	NE-CZ-NH2	-5.56	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	103	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	105	MET	CA-CB-CG	5.31	122.33	113.30
1	D	51	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	7	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	F	69	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	D	24	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	F	51	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	C	245	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1968	0	1932	17	0
1	B	1930	0	1895	13	0
1	C	1966	0	1943	15	0
1	D	2028	0	1962	12	0
1	E	1950	0	1901	7	0
1	F	1937	0	1888	16	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	4	0	6	0	0
2	D	8	0	12	0	0
2	E	8	0	12	0	0
2	F	8	0	12	1	0
3	A	146	0	0	2	0
3	B	150	0	0	1	0
3	C	145	0	0	0	0
3	D	156	0	0	1	0
3	E	178	0	0	0	0
3	F	155	0	0	0	0
All	All	12753	0	11587	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LEU:HD22	1:E:217:VAL:HG13	1.52	0.88
1:B:50:ASP:CB	3:B:544:HOH:O	2.34	0.74
1:A:97:GLU:HG3	1:A:152:ARG:NH2	2.10	0.67
1:C:7:ASP:O	1:C:24[B]:ARG:NH1	2.27	0.66
1:B:248:ARG:NH2	1:D:244:GLU:OE1	2.25	0.65
1:A:101:PRO:HD2	1:A:105:MET:SD	2.36	0.65
1:C:237:ILE:CG2	1:F:238:LEU:HD11	2.27	0.65
1:D:83:ARG:HB3	1:D:84:PRO:HD2	1.81	0.63
1:C:160[A]:VAL:HG11	1:C:188:LEU:HD12	1.82	0.62
1:B:248:ARG:HH22	1:D:244:GLU:CD	2.04	0.59
1:A:248:ARG:NH2	1:E:244:GLU:OE2	2.36	0.58
1:B:143:HIS:CG	1:B:150:ALA:HB2	2.40	0.56
1:C:238:LEU:HD11	1:F:237:ILE:CG2	2.37	0.55
1:B:160:VAL:HG11	1:B:188:LEU:HD12	1.88	0.54
1:B:146:ILE:HG22	1:B:146:ILE:O	2.08	0.54
1:E:143:HIS:CG	1:E:150:ALA:HB2	2.43	0.53
1:A:150:ALA:HB3	1:A:154:LEU:HD12	1.90	0.53
1:C:237:ILE:HG22	1:F:238:LEU:CD1	2.38	0.53
1:A:101:PRO:HG2	1:A:105:MET:HG3	1.91	0.52
1:B:146:ILE:HG12	1:C:259:PHE:CD1	2.44	0.52
1:C:238:LEU:HD12	1:F:237:ILE:HG22	1.92	0.52
1:B:99:THR:HG22	1:B:100:PRO:O	2.10	0.52
1:A:99:THR:HG22	1:A:100:PRO:O	2.10	0.51
1:B:171:LEU:HG	1:C:217:VAL:HG13	1.93	0.51
1:C:143:HIS:CG	1:C:150:ALA:HB2	2.46	0.51
1:C:238:LEU:CD1	1:F:237:ILE:HG22	2.42	0.50
1:A:28:LEU:HD11	1:A:62:ARG:NH1	2.28	0.49
1:A:217:VAL:HG13	1:C:171:LEU:HG	1.95	0.49
1:D:262:LYS:C	3:D:316:HOH:O	2.51	0.49
1:C:237:ILE:HG22	1:F:238:LEU:HD11	1.95	0.48
1:F:208:ILE:HD13	2:F:271:EDO:H11	1.95	0.48
1:D:213:ALA:CB	1:F:147:GLY:HA2	2.45	0.47
1:F:99:THR:HG22	1:F:100:PRO:O	2.15	0.47
1:C:238:LEU:CD1	1:F:237:ILE:CG2	2.93	0.46
1:B:238:LEU:HD11	1:D:237:ILE:CG2	2.46	0.45
1:A:238:LEU:HD22	3:A:289:HOH:O	2.16	0.44
1:A:247:LEU:HD21	3:A:466:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:GLY:HA2	1:F:213:ALA:CB	2.48	0.44
1:D:99:THR:HG22	1:D:100:PRO:O	2.17	0.44
1:F:24:ARG:HD3	1:F:24:ARG:HA	1.87	0.44
1:B:238:LEU:CD1	1:D:237:ILE:HG22	2.48	0.43
1:F:143:HIS:CG	1:F:150:ALA:HB2	2.54	0.43
1:D:213:ALA:HB3	1:F:147:GLY:HA2	2.00	0.43
1:E:99:THR:HG22	1:E:100:PRO:O	2.18	0.43
1:D:217:VAL:HG13	1:F:171:LEU:HG	2.01	0.42
1:A:213:ALA:CB	1:C:147:GLY:HA2	2.49	0.42
1:A:154:LEU:HD13	1:A:170:ALA:HB2	2.00	0.42
1:A:230:VAL:HG13	1:E:234:GLU:HG2	2.02	0.42
1:C:99:THR:HG22	1:C:100:PRO:O	2.21	0.41
1:A:171:LEU:HG	1:B:217:VAL:HG13	2.03	0.41
1:A:97:GLU:HG3	1:A:152:ARG:HH22	1.82	0.41
1:B:7:ASP:OD2	1:B:34:HIS:NE2	2.53	0.41
1:D:150:ALA:HB3	1:D:154:LEU:HD12	2.03	0.41
1:A:140:PHE:CD2	1:A:177:ARG:CD	3.04	0.41
1:A:245:ARG:NH2	1:E:244:GLU:OE1	2.54	0.40
1:F:140:PHE:CD2	1:F:177:ARG:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/274 (91%)	248 (99%)	2 (1%)	0	100	100
1	B	249/274 (91%)	247 (99%)	2 (1%)	0	100	100
1	C	251/274 (92%)	249 (99%)	2 (1%)	0	100	100
1	D	264/274 (96%)	259 (98%)	5 (2%)	0	100	100
1	E	250/274 (91%)	248 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	249/274 (91%)	247 (99%)	2 (1%)	0	100	100
All	All	1513/1644 (92%)	1498 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/227 (91%)	207 (100%)	0	100	100
1	B	198/227 (87%)	196 (99%)	2 (1%)	82	87
1	C	206/227 (91%)	203 (98%)	3 (2%)	72	78
1	D	207/227 (91%)	205 (99%)	2 (1%)	82	87
1	E	202/227 (89%)	202 (100%)	0	100	100
1	F	200/227 (88%)	197 (98%)	3 (2%)	72	78
All	All	1220/1362 (90%)	1210 (99%)	10 (1%)	86	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	ASP
1	B	260	VAL
1	C	69	ASP
1	C	250	GLU
1	C	263	ARG
1	D	7	ASP
1	D	69	ASP
1	F	7	ASP
1	F	69	ASP
1	F	263	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	ASN
1	C	48	ASN
1	D	48	ASN
1	E	48	ASN
1	F	44	HIS
1	F	48	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	271	-	3,3,3	0.58	0	2,2,2	0.33	0
2	EDO	A	272	-	3,3,3	0.57	0	2,2,2	0.03	0
2	EDO	B	271	-	3,3,3	0.57	0	2,2,2	0.73	0
2	EDO	B	272	-	3,3,3	0.37	0	2,2,2	0.31	0
2	EDO	C	271	-	3,3,3	0.46	0	2,2,2	0.80	0
2	EDO	D	271	-	3,3,3	0.36	0	2,2,2	0.78	0
2	EDO	D	272	-	3,3,3	0.51	0	2,2,2	0.80	0
2	EDO	E	271	-	3,3,3	0.43	0	2,2,2	0.80	0
2	EDO	E	272	-	3,3,3	0.70	0	2,2,2	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	F	271	-	3,3,3	0.48	0	2,2,2	0.53	0
2	EDO	F	272	-	3,3,3	0.58	0	2,2,2	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	271	-	-	0/1/1/1	0/0/0/0
2	EDO	A	272	-	-	0/1/1/1	0/0/0/0
2	EDO	B	271	-	-	0/1/1/1	0/0/0/0
2	EDO	B	272	-	-	0/1/1/1	0/0/0/0
2	EDO	C	271	-	-	0/1/1/1	0/0/0/0
2	EDO	D	271	-	-	0/1/1/1	0/0/0/0
2	EDO	D	272	-	-	0/1/1/1	0/0/0/0
2	EDO	E	271	-	-	0/1/1/1	0/0/0/0
2	EDO	E	272	-	-	0/1/1/1	0/0/0/0
2	EDO	F	271	-	-	0/1/1/1	0/0/0/0
2	EDO	F	272	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	271	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	253/274 (92%)	-0.20	3 (1%) 81 85	14, 21, 41, 58	0
1	B	252/274 (91%)	-0.04	8 (3%) 51 61	14, 24, 51, 72	0
1	C	252/274 (91%)	-0.08	3 (1%) 81 85	15, 24, 38, 58	0
1	D	266/274 (97%)	-0.09	8 (3%) 54 64	13, 22, 46, 58	0
1	E	254/274 (92%)	-0.25	0 100 100	13, 22, 35, 46	0
1	F	253/274 (92%)	-0.05	6 (2%) 62 71	13, 23, 43, 74	0
All	All	1530/1644 (93%)	-0.12	28 (1%) 71 79	13, 23, 43, 74	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	259	PHE	6.0
1	D	74	PRO	4.3
1	D	260	VAL	4.1
1	A	260	VAL	3.6
1	D	73	ILE	3.5
1	F	260	VAL	3.5
1	B	260	VAL	3.5
1	D	259	PHE	3.4
1	B	259	PHE	3.0
1	D	80	ILE	3.0
1	F	258	ALA	2.7
1	A	230	VAL	2.7
1	D	76	ASP	2.7
1	B	253	ALA	2.6
1	B	6	PHE	2.6
1	F	262	LYS	2.5
1	F	264	GLN	2.4
1	F	268	GLN	2.4
1	B	23	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	262	LYS	2.3
1	D	75	GLU	2.3
1	C	228	LEU	2.2
1	C	266	ASN	2.2
1	D	77	GLY	2.2
1	A	224	ILE	2.1
1	B	44	HIS	2.1
1	B	84	PRO	2.0
1	C	26	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	EDO	D	272	4/4	0.88	0.18	5.32	31,31,32,32	0
2	EDO	C	271	4/4	0.95	0.15	2.03	22,27,27,30	0
2	EDO	F	271	4/4	0.90	0.12	1.78	29,33,34,35	0
2	EDO	E	272	4/4	0.91	0.15	1.67	22,25,28,30	0
2	EDO	E	271	4/4	0.89	0.11	1.25	32,32,35,35	0
2	EDO	F	272	4/4	0.94	0.11	0.59	22,24,26,27	0
2	EDO	A	272	4/4	0.89	0.12	0.58	42,43,44,48	0
2	EDO	B	272	4/4	0.94	0.08	-0.47	32,34,34,35	0
2	EDO	D	271	4/4	0.96	0.07	-1.58	20,23,23,25	0
2	EDO	B	271	4/4	0.95	0.08	-1.84	24,29,31,35	0
2	EDO	A	271	4/4	0.97	0.08	-2.03	19,23,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.